

# Spin-orbit Coupling in Multilayer Superconductors with Charge Imbalance

Daisuke MARUYAMA\*, Manfred SIGRIST<sup>1</sup>, and Youichi YANASE<sup>2</sup>

*Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan*

<sup>1</sup>*Theoretische Physik, ETH-Honggerberg, 8093 Zurich, Switzerland*

<sup>2</sup>*Department of Physics, Niigata University, Niigata 950-2181, Japan*

This study investigates the spin susceptibility in the superconducting state of a multilayer system with a layer dependent Rashba spin-orbit coupling, representing a locally non-centrosymmetric superconductor. It is shown that the charge imbalance between the different layers yields a strong layer dependence in the susceptibility, most significantly for weak spin-orbit coupling, which is in contrast to the situation with equally distributed charge. These results can be relevant for experimental test in multilayer high- $T_c$  cuprates as well as in superconducting CeCoIn<sub>5</sub>/YbCoIn<sub>5</sub> superlattices with more than two layers.

KEYWORDS: superconductivity without local inversion symmetry, multilayer superconductor, spin susceptibility

Since the discovery of superconductivity in the heavy-fermion compound without inversion symmetry, CePt<sub>3</sub>Si,<sup>1)</sup> the non-centrosymmetric superconductivity has been studied extensively.<sup>2)</sup> Subsequently, several new non-centrosymmetric superconductors with unique properties have identified among heavy-fermion materials<sup>3-6)</sup> and others.<sup>7-12)</sup> Many exotic properties induced by the antisymmetric spin-orbit coupling have been studied in various contexts, such as the exotic superconductivity and spintronics.<sup>2)</sup>

On the other hand, many other superconductors lack local inversion symmetry even while having the global inversion symmetry in the crystal structure. In contrast to the uniform antisymmetric spin-orbit coupling in non-centrosymmetric systems, the antisymmetric spin-orbit coupling appears in such systems with special unit cell structures locally losing inversion symmetry. An interesting class of such “locally non-centrosymmetric system” is the multilayer systems in which the Rashba-type spin-orbit coupling is induced by the local violation of mirror symmetry.<sup>13)</sup> For instance, the recent experiment discovered superconductivity in the artificial superlattices of heavy-fermion superconductor CeCoIn<sub>5</sub> and conventional metal YbCoIn<sub>5</sub>,<sup>14)</sup> in which the superconductivity is induced by the multilayers of CeCoIn<sub>5</sub>. The multilayer high- $T_c$  cuprates represent a further example of superconductors where this type of spin-orbit coupling could play a role.<sup>15-17)</sup>

We investigated previously the basic properties of multilayer superconductors, such as the electron structure, superconducting order parameters, and magnetic properties with focus on the effects of Rashba spin-orbit coupling arising from the local non-centrosymmetry. It has been shown that the Rashba spin-orbit coupling significantly affects the superconductivity when the spin-orbit coupling is larger than the interlayer single particle hopping. Indeed, anomalous behavior of the upper critical field has been experimentally observed in the superlattice of CeCoIn<sub>5</sub> possibly connected with the paramagnetic limiting influenced by spin-orbit coupling.<sup>18)</sup> Several other superconductors with locally non-centrosymmetric crystal structure have been theoretically investigated.<sup>19-24)</sup>

In our earlier studies we focused on the superlattice of CeCoIn<sub>5</sub>,<sup>13)</sup> we neglected the difference of electric potential

between the inner and outer layers. This approximation may be valid for the superlattices of CeCoIn<sub>5</sub> since both interlayer hopping and Rashba spin-orbit coupling can be larger than the potential difference. On the other hand, it has been shown that the charge imbalance due to the potential difference plays an important role for the magnetism and superconductivity in high- $T_c$  cuprates with more than two layers.<sup>15-17,25)</sup> Thus, it is desirable to clarify the effect of spatially inhomogeneous Rashba spin-orbit coupling on multilayer superconductors with charge imbalance. For this purpose, we study the trilayer systems with charge imbalance for simplicity.

First, we introduce a model Hamiltonian for two-dimensional trilayer superconductors including spatially modulated Rashba spin-orbit coupling as

$$H = \sum_{m=1}^3 \left\{ \sum_{\mathbf{k},s} \varepsilon(\mathbf{k}) c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}sm} + \sum_{\mathbf{k},s,s'} \alpha_m \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{ss'} c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}s'm} \right. \\ \left. + \frac{1}{2} \sum_{\mathbf{k},s,s'} [\Delta_{ss'm}(\mathbf{k}) c_{\mathbf{k}sm}^\dagger c_{-\mathbf{k}s'm}^\dagger + \text{h.c.}] \right\} \\ + t_\perp \sum_{\mathbf{k},s,\langle m,m' \rangle} c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}sm'} + V \sum_{\mathbf{k},s} c_{\mathbf{k}s2}^\dagger c_{\mathbf{k}s2}, \quad (1)$$

where  $c_{\mathbf{k}sm}$  ( $c_{\mathbf{k}sm}^\dagger$ ) is the annihilation (creation) operator for an electron with spin  $s$  on a layer  $m$ . Two outer layers are denoted by  $m = 1, 3$ , while the inner layer is  $m = 2$ . We consider a simple square lattice and assume the dispersion relation as,  $\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - \mu$ . We choose the unit of energy as  $t = 1$  and fix the chemical potential  $\mu = -1$ , which leads to the electron density per site being approximately 0.63 for  $V = 0$ . The second term describes the Rashba spin-orbit coupling arising from the lack of local inversion symmetry. The coupling constants  $\alpha_m$  should be  $(\alpha_1, \alpha_2, \alpha_3) = (\alpha, 0, -\alpha)$  owing to the symmetry. We assume a simple Rashba-type form of  $\mathbf{g}$ -vector  $\mathbf{g}(\mathbf{k}) = (-\sin k_y, \sin k_x, 0)$  without going into microscopic derivation of the antisymmetric spin-orbit coupling.<sup>26)</sup>

The third term introduces intralayer Cooper pairing via an off-diagonal mean field. We ignore interlayer pairing as we assume a weak interlayer coupling. Owing to the spatially modulated Rashba spin-orbit coupling arising from the broken lo-

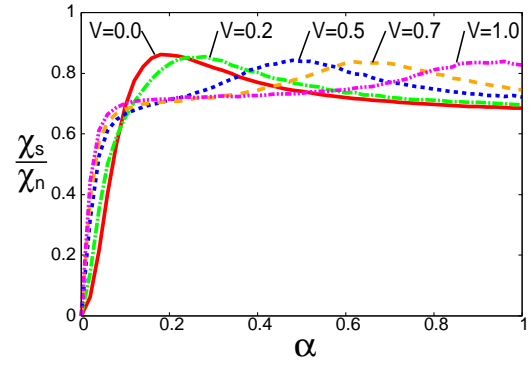
cal inversion symmetry, the order parameter  $\Delta_{ss'm}(\mathbf{k})$  involves both spin singlet and spin triplet components. One of the spin singlet and triplet components has the same sign between layers, while the other should change the sign. For instance, the staggered order parameter of p-wave superconductivity is induced by the staggered Rashba spin-orbit coupling when the d-wave Cooper pairing is predominant as in high- $T_c$  cuprates and CeCoIn<sub>5</sub>. We here neglect this spin triplet component because the spin susceptibility discussed below is independent of the staggered order parameter as we showed in ref. 13. In this paper, we assume the uniform spin singlet order parameter with s-wave symmetry ( $\Delta_{\uparrow\downarrow m}(\mathbf{k}) = -\Delta_{\downarrow\uparrow m}(\mathbf{k}) = \psi$ ) for simplicity. We have confirmed that the model for the d-wave superconductivity gives the qualitatively same results. We take  $|\psi| = 0.01$  to be sufficiently small to satisfy the condition  $|\Delta_{ss'm}(\mathbf{k})| \ll |\alpha_m| \ll \varepsilon_F$  ( $\varepsilon_F$  is the Fermi energy), as realized in most (locally) non-centrosymmetric superconductors.

The fourth term in eq. (1) describes the interlayer hopping of electrons between nearest-neighbor layers. Since we consider a quasi-two-dimensional system, we assume an interlayer hopping  $t_{\perp} = 0.1$  is much smaller than the intralayer hopping  $t = 1$ . In the following calculations, we will always use this value for  $t_{\perp}$ , if not stated otherwise. The last term of eq. (1) is the static potential  $V$  which induces the charge imbalance between the layers. We focus on the effect of the potential  $V$  in the following part. Note that the electron density per site in the inner layer is  $n_{\text{in}} \simeq 0.78, 0.68, 0.62, 0.56$ , and  $0.49$  for  $V = -0.5, -0.2, 0, 0.2$ , and  $0.5$ , respectively, while that in the outer layers is  $n_{\text{out}} \sim 0.63$  independent of  $V$ .

We calculate the spin susceptibility for magnetic fields along  $c$ -axis. The normalized spin susceptibility  $\chi_s/\chi_n$  for various potentials  $V$  and spin-orbit couplings  $\alpha$  are shown in Fig. 1, where  $\chi_s$  and  $\chi_n$  are the spin susceptibility at  $T = 0$  in the superconducting state and in the normal state, respectively. The normalized spin susceptibility along  $ab$ -plane is only half of that along  $c$ -axis as shown in ref. 13. For  $V = 0$ , our calculation reproduces the results obtained in ref. 13. The spin susceptibility vanishes  $\chi_s/\chi_n = 0$  for  $\alpha = 0$  as in the centrosymmetric spin singlet superconductors. With increasing  $\alpha$ , the spin susceptibility first ascends and shows a peak around  $\alpha \sim t_{\perp}$ , indicating the interplay between spin-orbit coupling  $\alpha$  and interlayer hopping  $t_{\perp}$ . Indeed, this is the fingerprint of crossover from the centrosymmetric superconductivity to the non-centrosymmetric superconductivity which occurs with increasing the spin-orbit coupling  $\alpha$ .<sup>13)</sup>

When we switch on the potential  $V$ , the peak of spin susceptibility shifts to  $\alpha \sim V$ . This shift does not mean the suppression of the Rashba spin-orbit coupling. Indeed, for a small spin-orbit coupling  $\alpha < t_{\perp}$ , the spin susceptibility in the superconducting state is significantly enhanced by the potential difference  $V$ . This indicates that the effect of Rashba spin-orbit coupling is enhanced by the charge imbalance for reasons discussed below.

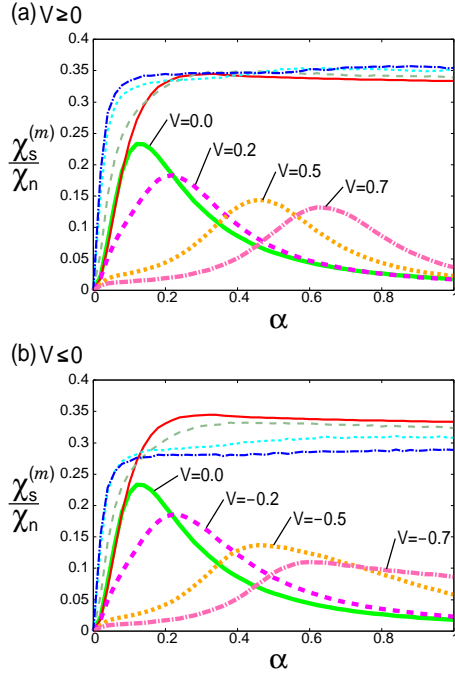
In order to elucidate roles of the charge imbalance in more details, we show the contribution of each layer to the spin susceptibility in Fig. 2. We assume the positive and negative potential  $V$  in Figs. 2(a) and 2(b), respectively. First, we discuss the small spin-orbit coupling  $\alpha < t_{\perp}$ . We see that the spin susceptibility of outer layers is enhanced by the charge



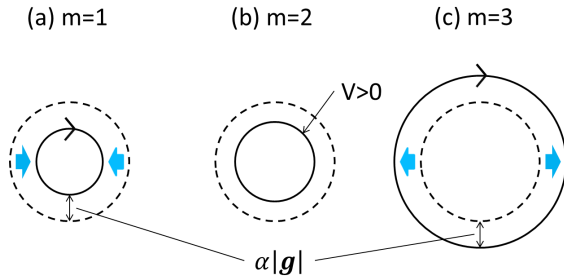
**Fig. 1.** (Color online) Spin susceptibility in the superconducting state at  $T = 0$  as a function of the spin-orbit coupling  $\alpha$ . We show the spin susceptibility along  $c$ -axis normalized by that in the normal state. We assume  $V = 0$  (solid line),  $V = 0.2$  (dashed-dotted line),  $V = 0.5$  (dotted line),  $V = 0.7$  (dashed line), and  $V = 1.0$  (dash two-dotted line), respectively.

the spin susceptibility shows a substantial layer dependence for the moderate potential difference  $V = 0.2$ , while the spin susceptibilities of inner and outer layers are nearly identical for  $V = 0$  and  $\alpha < t_{\perp}$ . This layer dependence appears through the decoupling of outer and inner layers due to the charge imbalance. As the potential difference  $|V|$  increases, the interlayer hybridization due to  $t_{\perp}$  is suppressed. Then, the effect of Rashba spin-orbit coupling is enhanced, and therefore, the spin susceptibility of the outer layers increases while that of inner layer decreases. When the layers are completely decoupled from each other, the spin susceptibility of the outer layers is not suppressed by the superconductivity as for uniformly non-centrosymmetric superconductors<sup>27)</sup> while that of the inner layer is completely suppressed as in the centrosymmetric superconductor. The total spin susceptibility shown in Fig. 1 is enhanced by the potential difference  $|V|$  since the contribution from the outer layers is larger than that from the inner layer.

Next, we discuss the large spin-orbit coupling  $\alpha > t_{\perp}$ . We see the peak of the spin susceptibility around  $\alpha \sim |V|$  in Fig. 1. This peak indicates the crossover in the electronic state. In order to illustrate this crossover, we show the schematic figures of Fermi surfaces for  $t_{\perp} = 0$  (see Fig. 3). The Fermi surface is identical for all layers at  $V = \alpha = 0$  as shown by the dashed lines in Fig. 3. When the potential of inner layer  $V > 0$  is turned on, the Fermi surface of the inner layer shrinks, as shown by the solid line in Fig. 3(b). Then, the mismatch of Fermi surfaces between  $m = 1$  and  $m = 2$  and between  $m = 2$  and  $m = 3$  suppresses the interlayer hybridization. When we switch on the Rashba spin-orbit coupling, the Fermi surfaces of the outer layers are split. One of the split Fermi surfaces having a positive spin helicity is drawn by the solid lines in Figs. 3(a) and 3(c), respectively. The Fermi surface of  $m = 1$  layer shrinks while that is enlarged for  $m = 3$ , because the spin-orbit coupling has the opposite sign  $\alpha_1 = -\alpha_3$ . Then, the mismatch of Fermi surfaces between  $m = 1$  and  $m = 2$  is removed, and therefore, the quasiparticle strongly hybridizes between the inner layer  $m = 2$  and the outer layer  $m = 1$ . This hybridization enhances the spin susceptibility of inner layer without decreasing the spin susceptibility of outer layers, as shown in Fig. 2. This is the reason why the total spin susceptibility shows a peak around  $\alpha \sim |V|$ . When the spin-orbit



**Fig. 2.** (Color online) Contribution of inner and outer layers to the spin susceptibility for (a) positive potential  $V$  and (b) negative potential  $V$ , respectively. Thin and thick lines show the spin susceptibility of outer layer and inner layer, respectively. We show the results for  $V = 0$  (solid line),  $|V| = 0.2$  (dashed line),  $|V| = 0.5$  (dotted line), and  $|V| = 0.7$  (dash-dotted line), respectively.



**Fig. 3.** (Color online) Schematic figure of Fermi surfaces in the absence of interlayer hopping  $t_{\perp} = 0$ . We show one of the split Fermi surfaces in the outer layers. The dashed lines show the Fermi surfaces for  $\alpha = 0$  and  $V = 0$ . The solid lines show the Fermi surface of  $m = 1, 3$  for  $\alpha > 0$  and that of  $m = 2$  for  $V > 0$ .

coupling  $\alpha$  is furthermore increased, the interlayer hybridization is suppressed again, and then the spin susceptibility of the inner layer is decreased.

In order to substantiate this picture, we now show the single particle wave function in the normal state. We focus on the single particle state with momentum  $\mathbf{k} = (0, k_F)$  and takes the  $x$ -axis for the quantization axis of spin, as in ref. 13. Then, the single particle Hamiltonian is block-diagonalized with the block

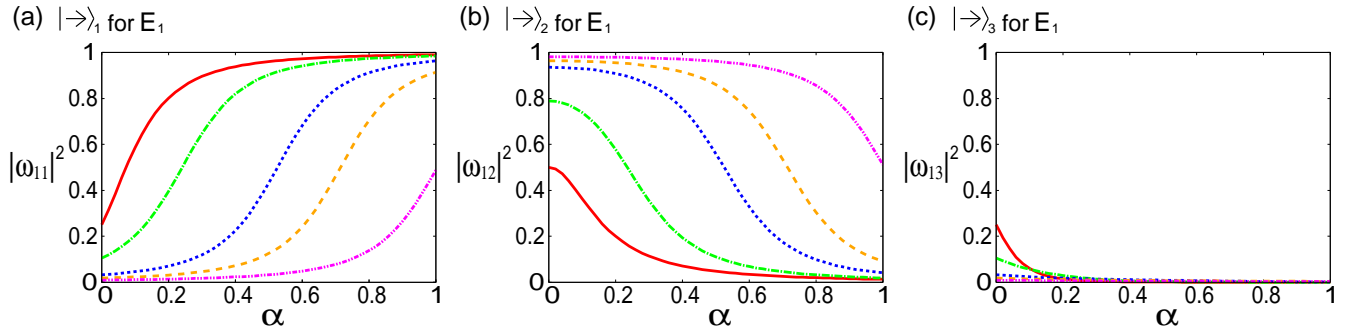
$$\begin{pmatrix} \varepsilon(\mathbf{k}) + \alpha|\mathbf{g}(\mathbf{k})| & t_{\perp} & 0 \\ t_{\perp} & \varepsilon(\mathbf{k}) + V & t_{\perp} \\ 0 & t_{\perp} & \varepsilon(\mathbf{k}) - \alpha|\mathbf{g}(\mathbf{k})| \end{pmatrix} \text{ for } \begin{pmatrix} |\rightarrow\rangle_1 \\ |\rightarrow\rangle_2 \\ |\rightarrow\rangle_3 \end{pmatrix}, \quad (2)$$

in the subspace of states describing the electrons on layer  $m$  with spin pointing in positive  $x$ -direction. Diagonalizing

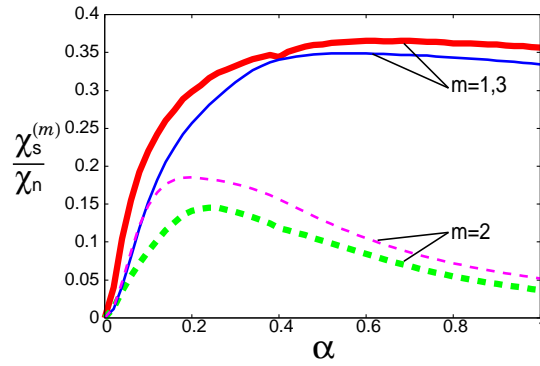
the  $3 \times 3$  matrix, we obtain three bands with the energy  $E_1(\mathbf{k}) > E_2(\mathbf{k}) > E_3(\mathbf{k})$  for the given  $\mathbf{k}$ -vector and wave function  $|j, \rightarrow\rangle = \sum_m \omega_{jm} |\rightarrow\rangle_m$  where  $j$  is the band index. Figure 4 shows the representative weights  $|\omega_{jm}|^2$  for the band  $j = 1$  on the three layers  $m$ . For vanishing spin-orbit coupling ( $\alpha = 0$ ) the single particle weight is localized on one to the layers for finite  $V$ , i.e. on the inner layer  $m = 2$  in the case of band  $j = 1$ . As the spin-orbit coupling is turned on, the layers begin to hybridize leading to the strongest hybridization for  $\alpha \sim V$  (strongest change of weight). Eventually, at larger  $\alpha$  the weight has shifted to the layer  $m = 1$ . Most notably, for the strongest hybridization between outer and inner layers, the effect of spin-orbit coupling is also transferred to the inner layer giving rise to a maximum of the susceptibility.

Charge imbalance may open a way to observe "local non-centrosymmetry" in multilayer superconductors such as high- $T_c$  cuprates even for comparatively weak spin-orbit coupling by studying the local spin susceptibility. The local spin susceptibility is, in principle, accessible in site-selective NMR experiment through Knight shift measurements.<sup>15–17</sup> Experimental investigations have not focused on the aspect of local non-centrosymmetry so far. In order to motivate such studies, we consider here a simple tight-binding model as an approximation to generic band structure of trilayer high- $T_c$  cuprates in the overdoped regime in order to avoid complications with antiferromagnetic order. The inplane hopping involves nearest- and next-nearest-neighbor hopping, leading to  $\varepsilon(\mathbf{k}) = -2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y - \mu$  and the interlayer hopping  $t_{\perp}$  is simply nearest neighbor. Experimental studies give for such systems a charge distribution among the layers of  $n_{\text{in}} \simeq 0.9$  and  $n_{\text{out}} \simeq 0.8$ .<sup>17</sup> These values are obtained by the choice of parameters  $(t_1, t_2, t_{\perp}, \mu, V) = (1, 0.3, 0.1, -1.08, -0.2)$  which we now use to calculate the spin susceptibility in the superconducting phase for varying  $\alpha$  as depicted in Fig. 5. We find a clear difference in the spin susceptibility between inner and outer layers even for small spin-orbit coupling  $\alpha < 0.04$ . This is in contrast with the result for  $V = 0$ . Thus, the moderate charge imbalance in our model for multilayer cuprates significantly enhances the effect of Rashba spin-orbit coupling on outer layers. Naturally the Rashba spin-orbit coupling would also play a role for the antiferromagnetic and superconducting states of multilayer cuprates. In particular, the difference of magnetic response between outer and inner layers would affect the superconducting phase structure in the magnetic field. For example, the pair-density wave state which has been discussed recently<sup>28</sup>) would be stabilized by the reduced interlayer hybridization due to the cooperation of spin-orbit coupling and charge imbalance. A more detailed discussion of the interplay of magnetism and superconductivity in the high- $T_c$  cuprates in the light of local non-centrosymmetry will be given elsewhere.

In summary, we have investigated the effect of charge imbalance on the spin susceptibility of trilayer superconductors by taking into account the Rashba spin-orbit coupling arising from the local non-centrosymmetry. As an important result, we find that charge imbalance enhances the spin susceptibility of outer layers, because the interlayer hybridization is suppressed by the mismatch of Fermi surfaces. The same effect leads to a reduction of the spin susceptibility of the inner layer. For a small spin-orbit coupling and moderate charge



**Fig. 4.** (Color online) Single particle weight  $|\omega_{jm}|^2$  of the band  $j=1$  on the layer (a)  $m=1$ , (b)  $m=2$ , and (c)  $m=3$ , respectively. We assume the potential on the inner layer  $V=0$  (solid lines),  $V=0.2$  (dash-dotted lines),  $V=0.5$  (dotted lines),  $V=0.7$  (dashed lines), and  $V=1$  (dashed two-dotted lines), respectively.



**Fig. 5.** (Color online) Spin susceptibility in the model for the multilayer high- $T_c$  cuprates. We show the spin susceptibility of inner (thick dashed line) and outer (thick solid line) layer for  $V = -0.2$ . The thin lines show the results for  $V = 0$ . The other parameters are described in the text.

layers, thus showing that the effect of spin-orbit coupling is enhanced by the charge imbalance. This may also be the case for multilayer high- $T_c$  cuprates. When the spin-orbit coupling is increased, the strong hybridization occurs between the inner and outer layers around  $\alpha \sim |V|$ , and then, the spin susceptibility of inner layer increases substantially. These cooperative and/or competing roles of Rashba spin-orbit coupling and charge imbalance can be tested by the experiments for multilayer superconductors such as the high- $T_c$  cuprates as well as the superlattice of  $\text{CeCoIn}_5/\text{YbCoIn}_5$ .

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